Naval Research Laboratory
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NRL/MR/5710--09-8895

Analysis of Silicon Nitride (Si_3N_4) for Use in a Small Recuperated Turboshaft Engine

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September 21, 2009

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
21-09-2009

2. REPORT TYPE
Memorandum Report

3. DATES COVERED *(From - To)*
08/11/2004 - 04/08/2005

4. TITLE AND SUBTITLE
Analysis of Silicon Nitride (Si_3N_4) for Use in a Small Recuperated Turboshaft Engine

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Richard L. Stark, Jr. and Michael J. Vick

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Naval Research Laboratory
4555 Overlook Avenue, SW
Washington, DC 20375-5320

8. PERFORMING ORGANIZATION REPORT NUMBER
NRL/MR/5710--09-8895

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Office of Naval Research
One Liberty Center
875 North Randolph St.
Arlington, VA 22203-1995

10. SPONSOR / MONITOR'S ACRONYM(S)
ONR/NRL

11. SPONSOR / MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
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15. SUBJECT TERMS
Oxidation, Silicon nitride, Ceramic, Volatilization, Small turbine

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
Unclassified	Unclassified	Unclassified	UL	7	Michael J. Vick
					19b. TELEPHONE NUMBER *(include area code)* (202) 767-5845

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

ANALYSIS OF SILICON NITRIDE (SI_3N_4) FOR USE IN A SMALL RECUPERATED TURBOSHAFT ENGINE

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ABSTRACT

This analysis was performed to determine whether Silicon Nitride (Si_3N_4) could be used as a material for the fabrication of the Small Recuperated Turboshaft Heavy Fuel Engine (SMART-HFE). Oxidation and volatilization of Silicon Nitride in the presence of water vapor has been an issue under the conditions of turbine combustion [1]. Through the use of previous research, the recession rates of Si_3N_4 were predicted for various operating conditions. The volatilization rate required by the SMART engine was chosen to be 1/4 mm per kilo-hour, the equivalent of the rotor blade tip clearance. The calculations made showed that Silicon Nitride (Si_3N_4) is an acceptable material for the use in the SMART-HFE combustion chamber and turbine.

INTRODUCTION

The purpose of this analysis was to determine whether Silicon Nitride (Si_3N_4) could be used as a material for the fabrication of the Small Recuperated Turboshaft Heavy Fuel Engine (SMART-HFE). Silicon Nitride is the optimum material choice for construction of the SMART-HFE combustion chamber and turbine. However, oxidation and volatilization of Silicon Nitride in the presence of water vapor has proven to be an issue under the conditions of turbine combustion [1]. Utilizing previous research, the recession rates of Si_3N_4 were predicted for various operating conditions.

The prediction of the oxidation and volatilization of Silicon Nitride was performed for a range of operating conditions. The pressures, temperatures and velocities used for the analysis were dictated by the performance specifications set by the SMART-HFE (Table 1).

The governing stoichiometric equation for the combustion of jet fuel (assumed to be $C_{12}H_{22}$) in air is the following:

$$\begin{aligned} &C_{12}H_{22} + 17.5(O_2 + 3.76N_2) \\ &\longrightarrow 11H_2O + 12CO_2 + 65.8N_2 \end{aligned} \tag{1}$$

The conditions required for SMART – HFE dictate that the air-fuel equivalence ratio be 7.6, which corresponds to the excess air reaction of:

$$\begin{aligned} &C_{12}H_{22} + 133O_2 + 500.08N_2 \\ &\longrightarrow 11H_2O + 12CO_2 + 500.08N_2 + 115.5O_2 \end{aligned} \tag{2}$$

The water vapor formed from Equation (2) results in the following oxidation reaction of the Silicon Nitride:

$$\begin{aligned} &Si_3N_4(s) + 6H_2O \\ &\longrightarrow 3SiO_2(s) + 2N_2(g) + 6H_2(g) \end{aligned} \tag{3}$$

Simultaneously, the volatilization of the Silica occurs by Equation (4).

$$SiO_2(s) + 2H_2O(g) \longrightarrow Si(OH)_4(g) \tag{4}$$

The oxidation and volatilization reaction have been previously modeled using paralinear kinetics [1, 2, 3]. The paralinear kinetic equations show that the reaction will reach a steady state after time t_L. At steady state conditions the oxide thickness and the recession rate of the Silica will remain constant, x_L and y_L [1]. Figure 1 shows a graphical representation of the paralinear model. Semiempirical

Manuscript approved January 25, 2006.

equations for the time constant, oxide thickness, and recession rate are given below [1]. The only required information to prove that Silicon Nitride is acceptable for a combustion environment is the recession rate, however all three paralinear kinetic terms are calculated here in order to provide a complete kinetic model.

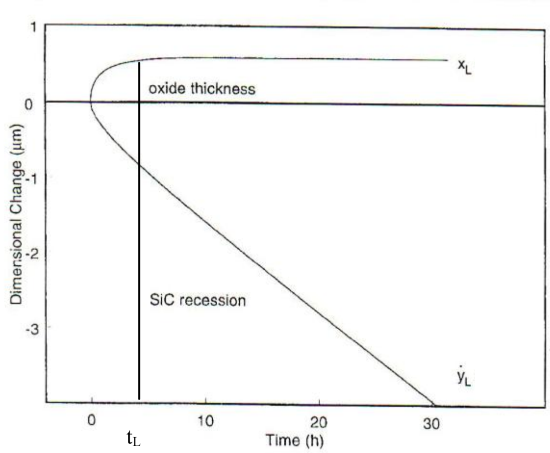

Figure 1. Paralinear kinetic oxidation and volatilization model for ceramics.

$$x_{L,1315C} = 0.615\frac{P_{tot}^{1/2}}{P_{H_2O}v}\mu \quad \text{(Oxide Thickness)} \quad (5)$$

$$t_{L,1315C} = 1.71\frac{P_{tot}}{P_{H_2O}^{3}v}\ \text{h} \qquad \text{(Time constant)} \quad (6)$$

$$y_{L,1315C} = 0.18\frac{P_{H_2O}^{2}v^{1/2}}{P_{tot}^{1/2}}\mu / h \quad \text{(Recession rate)} \quad (7)$$

The values calculated from Equations (5) – (7) are at a temperature of 1315 degrees Celsius. The values were modified to show temperature variation using the following proportions:

$$x_L \propto e^{\Delta H_{vol} - \Delta H_{ox}/RT} \qquad (8)$$

$$t_L \propto e^{2\Delta H_{vol} - \Delta H_{ox}/RT} \qquad (9)$$

$$y_L \propto e^{-\Delta H_{vol}\ /RT} \qquad (10)$$

The Oak Ridge National Laboratory has collected data measurements of the recession rates of Silica in water vapor [2, 3]. The data has been scaled according to pressure and velocity in order for comparison with the calculated oxidation and volatilization rates of Silicon Nitride.

RESULTS

The calculations for the recession rate of the Silicon Nitride were made using the pressures and velocity given by the SMART- HFE. Table 1 shows a summary of the flow conditions in the heavy fuel engine.

Table 1. SMART-HFE

Pressure (Water Vapor)	0.0413 atm
Pressure (Total)	2.4 atm
Maximum Velocity	400 m/s
Maximum Temperature	1250° C
Recession Rate	0.25 mm/kh

The limiting oxide thickness, time constant, and recession rate were calculated to be 1.15 µm, 144.6 h, and 0.00925 µm / h (mm/ kh) respectively. These values are calculated at temperatures of 1315° C. Figures (2) – (4) display the variation of the oxide thickness, time constant, and recession rate with respect to temperature. The assumed values of the enthalpy of reaction, ΔH_{vol} and ΔH_{ox} were 3 and 35 kJ/kmol[3]. These assumptions are fairly good for temperatures under 1400° C. It was also assumed that $Si(OH)_4$ was the major volatile species.

The data shows that the recession rate at 1250° C is 0.00925 mm /kh. This recession rate is less than 0.25 mm/kh and therefore acceptable for the SMART-HFE.

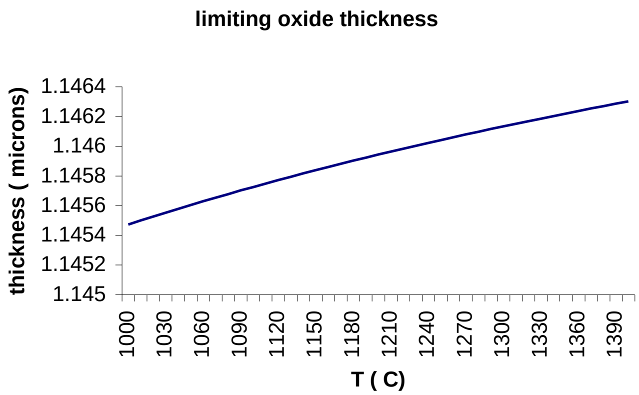

Figure 2. Limiting oxide thickness variation with temperature.

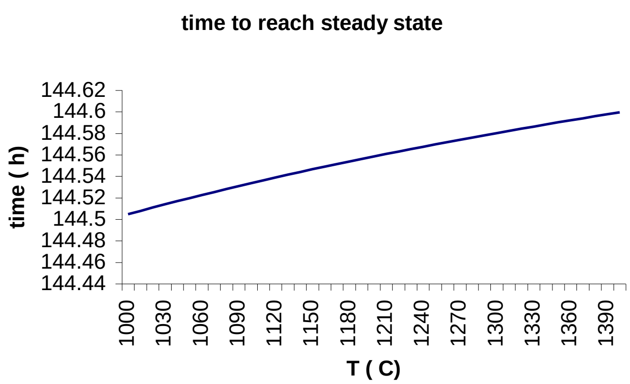

Figure 3. Steady state time constant variation with temperature.

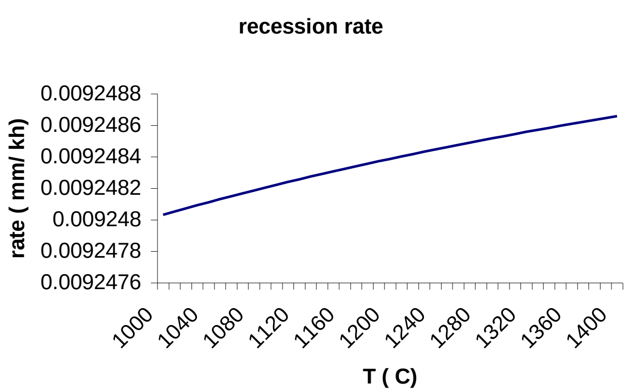

Figure 4. Recession rate variation with temperature.

Previously, the combustion intake air has been assumed to contain 0% humidity. However, this may not always be the case. The water contained in the ambient air will affect the recession of the Silica. The "worst case" operating scenario for SMART-HFE is 50° C and 100% humidity. The saturated pressure of water vapor at 50° C is equal to 12.349 kPa (100% humidity). This pressure is added to the pressure of water vapor for the combustion conditions, see Table 1. The resulting changes in x_L, t_L, and y_L can be seen in Figures (5) – (7). The recession rate has increased to 0.1472 mm/ kh.

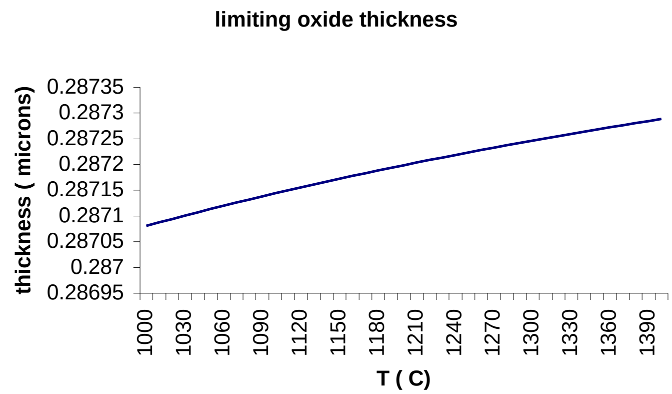

Figure 5. Limiting oxide thickness at 100 % humidity

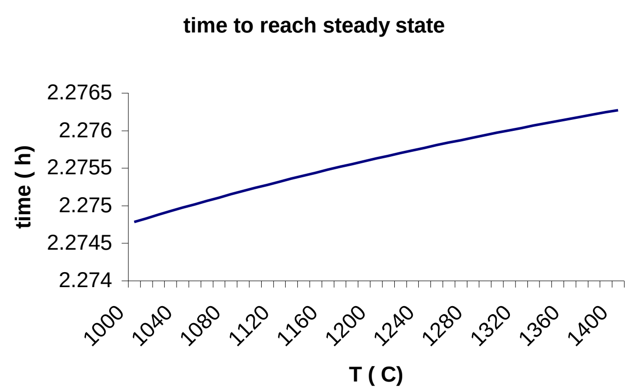

Figure 6. Time constant at 100 % humidity.

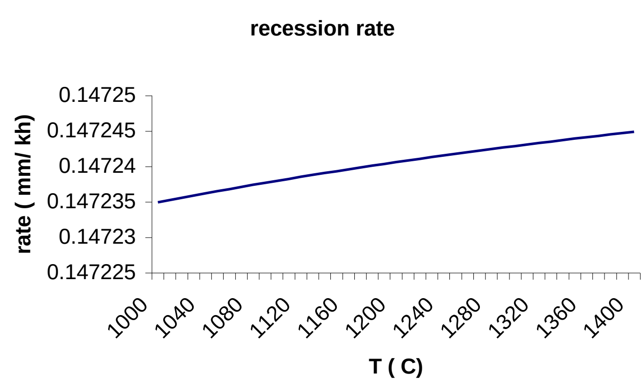

Figure 7. Silicon Nitride recession rates at 100 % humidity.

Experimental data, collected by the Oak Ridge National Laboratory and NASA Glenn, was used along with proportional constants to verify the calculated results [2, 3]. Equation (11) was used to scale the measured data, see Table 2.

$$y_L \propto \frac{v^{1/2} P_{H_2O}^2}{P_{total}^{1/2}} \tag{11}$$

$$y_L \propto k_L \tag{12}$$

Table 2. Experiment results for different Silicon Nitride alloys.

	CVD	SN282	AS800
$k_{L\ mg/cm^{\wedge}2\ h}$			
1200° C	$5.0 * 10^{-3}$	$9.8 * 10^{-4}$	$5.9 * 10^{-3}$
1400° C	$6.2 * 10^{-3}$	$1.8 * 10^{-3}$	$6.6 * 10^{-3}$

The following figures show the experimental data scaled to match the SMART-HFE operating conditions shown in Table 1. Figures 8, 9, and 10 correspond to 0 % humidity and Figures 11, 12, and 13 correspond to 100% humidity. A linear interpolation between 1200° C and 1400° C was used in order to gain information at the required temperature of 1250° C.

Note that the multiple lines show the variation with respect to velocity changes. The lower most line represents 50 m/s and the upper-most line represents 400 m/s. Each line is incremented by 10 m/s.

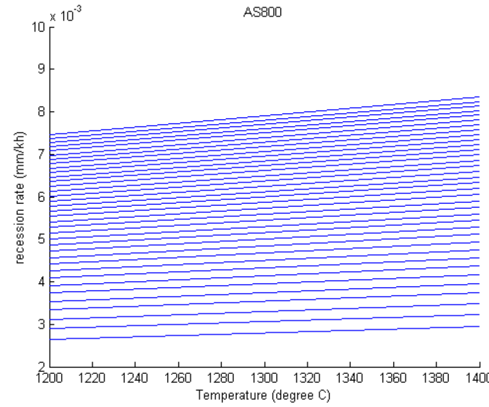

Figure 8. AS800 recession rates at 0 % humidity.

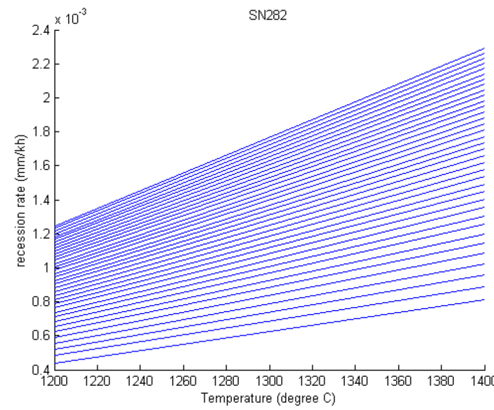

Figure 9. SN282 recession rates at 0 % humidity.

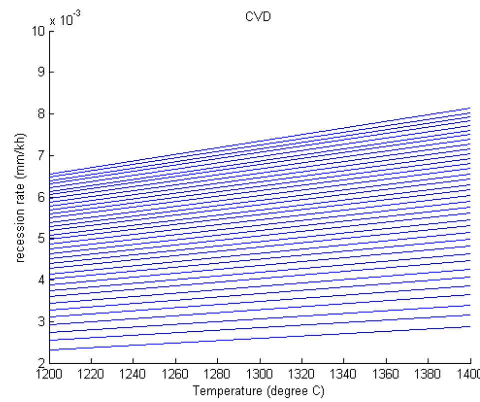

Figure 10. CVD recession rates at 0 % humidity.

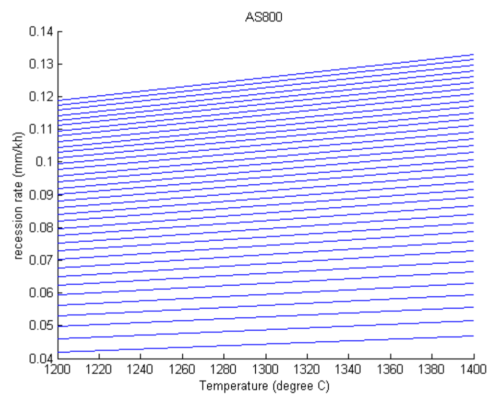

Figure 11. AS800 recession rates at 100 % humidity.

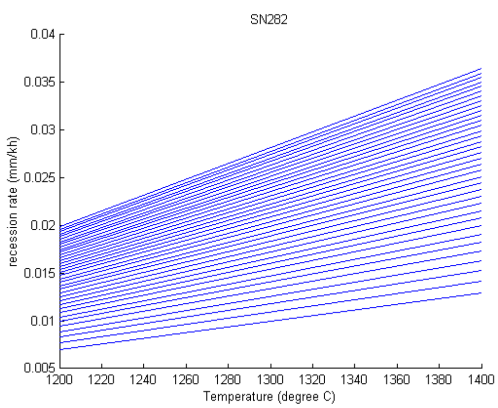

Figure 12. SN282 recession rates at 100 % humidity.

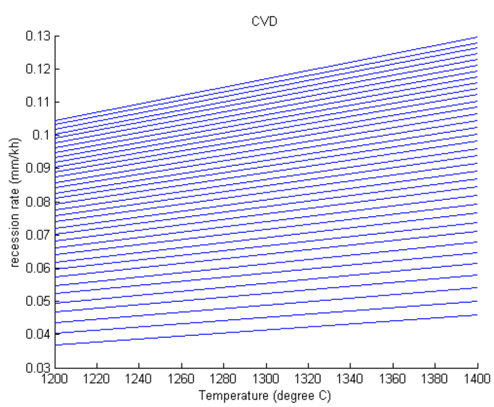

Figure 13. CVD recession rates at 100 % humidity.

The value of the recession rate for pure Silicon Nitride (CVD) at the SMART-HFE operating conditions is approximately 0.11 mm/kh. This is lower than the calculated value of 0.147 mm / kh. The SMART engine is required recession rate is 0.25 mm/kh, therefore the recession rate of 0.147 mm/ kh is acceptable. Silicon Nitride (Si_3N_4) is an appropriate material for the use in the SMART-HFE combustion chamber and turbine.

CONCLUSIONS

After analysis and calculations for the recession rates of Silicon Nitride under conditions set by SMART-HFE the following conclusions can be made:

1. After reaching steady- state at 100 % humidity, the "worst case" recession rate of Si_3N_4 will be approximately 0.147 mm / kh.
2. Silicon Nitride (Si_3N_4) is an acceptable material for the use in the SMART-HFE combustion chamber and turbine be because the calculated recession rate is less than 0.25 mm/kh.

ACKNOWLEDGMENTS

The U.S. Naval Research Laboratory is currently in the developmental stages of the design of a small recuperated turboshaft engine. The study was funded by the Office of Naval Research in collaboration with the Naval Research Laboratory.

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